A COMPUTER PROGRAM FOR BINARY MIXTURE CALCULATION

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INTRODUCTION

A computer program for binary mixture calculation has been developed by this Laboratory. The program calculates the percent composition of a binary mixture (component A and component B) provided both components contain a common ingredient, M. Components A and B can each contain other ingredients in addition to M. For best results, the amount of M present in each component should not be too similar. The program utilizes finding the values of M in the sample to determine the values of components A and B. Any combination of a two-component mixture could be determined using this program. An example of such a mixture is a Soybean Oil/Canola Oil combination where C18:2 (linoleic acid) is the common ingredient, M.

EXPERIMENTAL

Equipment

1. Use any analytical technique applicable such as High Pressure Liquid Chromatography, Gas Chromatography, Atomic Absorption Spectroscopy, Inductively Coupled Plasma Emission Spectroscopy, etc., to detect ingredient M.

2. Use the developed computer program, called mixture.exe, with any IBM or IBM-compatible computer employing the Microsoft Windows operating system to determine percent A and percent B in the binary mixture. The computer program is written in C computer language. A copy of the compiled program on diskette can be obtained by contacting the author.

Standards Preparation

For the binary mixture example given above in the **INTRODUCTION**, standards could be prepared as follows:

1. Purchase or have available pure Soybean Oil (A) and pure Canola Oil (B).

2. Prepare any number of standards, with each standard having a different combination of A and B, such as:

   a. Standard 1 : 100% A - 0% B

   b. Standard 2 : 70% A - 30% B

   c. Standard 3 : 40% A - 60% B

   d. Standard 4 : 0% A - 100% B

Data Acquisition

1. Analyze for M (in the case of this example, C18:2) in each of the standards using the chosen technique.

2. Analyze for M (in the case of this example, C18:2) in the sample using the chosen technique.

Procedure

1. Load the program, mixture.exe, on an IBM or IBM-compatible computer running with Microsoft Windows operating system.

2. Go to file manager.

3. Click on "mixture.exe" to initiate the program.

4. Follow the program prompts and enter your data as in Figure 1.

5. Enter output file name.

6. Print the output file.

RESULTS AND DISCUSSION

The program "mixture.exe" automatically calculates the results and creates an output file. The output file is a complete report including original data, standard linearity equation, calculations, and results. Executing the program "mixture.exe" is easy and convenient. No standard calibration curve is needed. Figure 1 demonstrates how the program is executed. Figure 2 shows a report in the output file. Figure 3 (4 pages) is a source file of the program, mixture.exe.

CONCLUSION

The program is a convenient way to determine the composition of a two-component mixture provided the components have a common ingredient. Familiarity with Microsoft Windows facilitates understanding the program.

```
Matter A in mixture:  Soybean Oil
Matter B in mixture:  Canola Oil
Detected Substance:   C18:2

How many standards?  4

Enter std 1 (%A):          0
        reading :                    10.88

Enter std 2 (%A):          6.9
        reading :                    13.22

Enter std 3 (%A):         14.7
        reading :                    16.67

Enter std 4 (%A):        100
        reading :                    51.38

How many samples?  1

Sample 1 number:  12345
        reading:  26.76

Output File Name:  mixture.out
```

Figure 1 - Executing the program "mixture.exe"

Assay for Mixture of Soybean Oil and Canola Oil

(1) Data:

	Soybean Oil(X)	Canola Oil	Reading(C18:2)
std 1	0.00	100.00	10.88
std 2	6.90	93.10	13.22
std 3	14.70	85.30	16.67
std 4	100.00	0.00	51.38
spl 1	X1	100-X1	26.76

(2) Standard linearity equation:

X	Y
0.00	10.88
6.90	13.22
14.70	16.67
100.00	51.38

Linearity Coefficient: = 0.9999
Linearity Equation: X = (Y - 10.644)/0.407

(3) Calculation:

X1 = (26.76 - 10.644)/0.407 = 39.55

(4) Results:

12345: 39.55% Soybean Oil and 60.45% Canola Oil

Figure 2. A report in output file "mixture.out."

```
/* Frank Hue */
/* 10-23-95 */
/* mixture.cpp */

#include <stdio.h>
#include <math.h>

int main(void)
{
 float  X[20],Y[20],Dx[20],Dy[20],data[20],result[20],
     Ma[20],Mb[20],Rspl[20],R,S,T,P,Sx,Sy,Ax,Ay,E,a,b;
 int  M,N,I;
 char Ds[20],filename[12], Num[20][20];
 FILE *outf;

 printf("Matter A in mixture : ");
 scanf("%s", &Ma);
 printf("Matter B in mixture : ");
 scanf("%s", &Mb);
 printf("Detected substance : ");
 scanf("%s", &Ds);
 printf("\nHow many standard data ? ");
 scanf("%d", &N);
 printf("\n");

 Sx = 0;
 Sy = 0;
 for (I = 1; I <= N; I++)
   {
    printf("Enter std %d (%A)  :         ", I);
    scanf("%f", &X[I]);
    printf("            (reading):              ");
    scanf("%f",&Y[I]);

    Sx = Sx + X[I];
    Sy = Sy + Y[I];
   }
```

Figure 3(a) - The source file of program "mixture.exe."

```
Ax = Sx / N;
Ay = Sy / N;

R = 0;
S = 0;
T = 0;
for (I = 1; I <= N; I++)
  {
   Dx[I] = X[I] - Ax;
   Dy[I] = Y[I] - Ay;
   R = R + Dx[I] * Dy[I];
   S = S + Dx[I] * Dx[I];
   T = T + Dy[I] * Dy[I];
  }

E = 0.5 * log(S * T);
P = R /exp(E);
b = R / S;
a = Ay - b * Ax;

printf("\nHow many samples ? ");
scanf("%d",&M);

for (I = 1; I <= M; I++)
  {
   printf("\nSample %d Number: ", I);
   scanf("%s", &Num[I]);
   printf("        reading: ");
   scanf("%f", &Rspl[I]);

   result[I] = (Rspl[I] - a) / b;
  }
printf("\nOutput File Name : ");
scanf("%s", &filename);
outf = fopen(filename, "w");
```

Figure 3(b) - The source file of program "mixture.exe."

```
fprintf(outf, "\n\n\n          Assay for Mixture of %s and
    %s\n", &Ma,&Mb);
 fprintf(outf, "
==============================================");

 fprintf(outf, "\n\n\n(1) Data : \n");
 fprintf(outf, "     ----   \n");
 fprintf(outf, "            %s(X)    %s       reading(%s)\n\n",
        Ma, Mb, Ds);

 for (I = 1; I <= N; I++)
   {
    fprintf(outf, "     std %d    %6.2f        %10.2f
           %12.2f\n", I,X[I],100-X[I],Y[I]);
   }
 fprintf(outf, "\n");
 for (I = 1; I <= M; I++)
   fprintf(outf, "     spl %d        X%d            100-X%d
          %12.2f\n", I, I, I,Rspl[I],data[I]);

 fprintf(outf, "\n\n(2) Standard linearity equation :\n");
 fprintf(outf, "     ---------------------------\n");
 fprintf(outf, "\n         X            Y\n");
 fprintf(outf, "        ---          ----\n");
 for (I = 1; I <= N; I++)
   fprintf(outf, "    %7.2f        %6.2f\n", X[I],Y[I]);

 fprintf(outf, "\n     Linearity Coefficient = %6.4f", P);
 fprintf(outf, "\n     Linearity Equation:  X = (Y -
        %6.3f)/%6.3f = %5.1f",a,b,result[I]);

 fprintf(outf,"\n\n\n(3) Calculation: \n");
 fprintf(outf,"     -----------");
 for (I = 1; I <= M; I++)
   fprintf(outf,"\n\n     X%d = (%5.2f - %6.3f)/%6.3f",
          I,Rspl[I],a,b);
```

Figure 3(c) - The source file of program "mixture.exe."

```
 fprintf(outf, "\n\n\n(4) Results: \n");
 fprintf(outf, "     -------\n");

 for (I = 1; I <= M; I++)
   {
    fprintf(outf, "\n     %s :", Num[I]);
    fprintf(outf, "    %5.2f% ", result[I]);
    fprintf(outf, "%s and ", Ma);
    fprintf(outf, "%5.2f% ", 100-result[I], Mb);
    fprintf(outf, "%s.\n", Mb);
   }
 fclose(outf);
 return 0;
}
```

Figure 3(d) - The source file of program "mixture.exe."